

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.03e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.98e-01

Confidence level: 5.37e-01

Nearest Neighbors from the Training Set

Image not found

Idoxuridine

Measured: 5.65e-03

Predicted: 9.97e-03

Image not found

Imazaquin

Measured: 2.89e-04

Predicted: 4.03e-03